

The Dortmund Databank (DDB) - A Comprehensive Database for Thermophysical Properties

W. Cordes^S and J. Menke
DDBST GmbH
Industriestraße 1
26121 Oldenburg Germany

K. Fischer, J. Rarey, and J. Gmehling^C
Industrial Chemistry
Carl von Ossietzky Universität Oldenburg
26111 Oldenburg Germany
gmehling@tech.chem.uni-oldenburg.de

In 1973 a computerized data bank for phase equilibrium data was started at the University of Dortmund with a view towards the synthesis and design of separation processes, fitting and critical examination of model parameters used for process simulation, and the development of group contribution methods. In the beginning mainly VLE data for non-electrolyte mixtures ($T_b > 0\text{ }^{\circ}\text{C}$) were considered; later on also VLE (including compounds with $T_b < 0\text{ }^{\circ}\text{C}$), LLE, h^E , γ^{∞} , azeotropic, c_p^E , SLE, v^E , adsorption equilibrium,... data for non-electrolyte and electrolyte systems as well as pure component properties were stored in a computer readable form. This data bank (Dortmund Data Bank (DDB)) now contains nearly all worldwide available phase equilibrium data, excess properties and pure component properties.

To use the full potential of this comprehensive compilation a powerful software package was developed by DDBST GmbH (www.ddbst.de) for verifying, storing, handling and processing the various pure component and mixture data. Programs for the correlation and prediction of pure component properties, phase equilibria, excess properties as well as graphical data representation were also included.

Together with the data from the Dortmund Data bank these programs allow the analysis of the real mixture behavior of a system of interest and the ability to fit reliable model parameters (g^E -models, equations of state, group contribution methods) for the synthesis and design of chemical processes on the basis of the most actual experimental data and estimation methods.

In addition, especially the data banks for γ^{∞} , azeotropic data, LLE and VLE serve as ideal sources for e.g. the selection of suitable solvents for azeotropic or extractive distillation, extraction, absorption.

The talk will give an overview on the development, structure and contents of the DDB and will highlight certain aspects of the accessibility and use of thermophysical data in the Internet age. Future plans concerning the development of the DDB and the software package DDBSP will be discussed.

Besides the lecture, program demonstrations are available on request.